REMARKS

Applicants amend claims 1, 5, and 9 to clarify that which was already implicit in the claims, and add claims 28-35. As a result, claims 1, 5, 9, and 13-35 are pending, the remaining claims having been withdrawn from consideration. Support for claims 28-35 may be found at least on pages 7-9 and in Figs. 3-4.

Rejection of Claims Under 35 U.S.C. 102(b)

The Examiner rejected claim 1 under 35 U.S.C. § 102(b) as being anticipated by Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis," Purdue University 1993 ("Helson thesis"). In response to the Examiner's rejection, Applicant has amended claim 1 to recite "laying out symmetrically equivalent atoms and bonds in [a] chemical structure diagram in accordance with the identified symmetry" instead of "positioning..." in order to emphasize the active nature of the step in which symmetry is used to generate the chemical structure diagram. [emphasis added] We explain this in more detail below.

As previously noted in our Response dated May 21, 2007, the Helson thesis does not disclose positioning or "laying out symmetrically equivalent atoms and bonds in [a] chemical structure diagram in accordance with the identified symmetry," as required by amended claim 1. [emphasis added] Rather, the Helson thesis is concerned with the perception of symmetry.

According to the present specification, laying out a structure diagram involves at least two distinct steps. In the first step, symmetry in a molecule is perceived. In the second, quite distinct, step, the perceived symmetry in the chemical structure is used during the laying out of the chemical structure diagram so as to reflect the perceived symmetry in the resulting diagram. The present specification provides insight as to what the second, layout step means:

> ...when a diagram is to be produced for a molecule, symmetry inherent in the molecule is perceived, and during layout of the structure diagram, representations of atoms and bonds are positioned to express the perceived symmetry. (page 6, line 18 to page 7, line 2) [emphasis added]

How positioning takes account of the perceived symmetry depends on the type of symmetry that is perceived:

> When an atom or bond is positioned during the assembly phase ... attention is paid to whether the atom or bond belongs to one of the determined instances of symmetry... If the type of symmetry involved is reflection ... the other atom or bond is placed on the opposite side of the mirror line that runs through the pivot point of the group in the instance.... If the type of symmetry involved is rotation, the symmetrically equivalent atoms or bonds are positioned at appropriate rotational points, based on the pivot point. (page 9, lines 1-12) [emphasis added]

In other words, the chemical structure diagram layout step, though it takes as input the perceived symmetry in the molecule, is by no means a part of the symmetry perception step. Indeed, traditional chemical structure algorithms generally start with one atom of a chemical structure and then lay out its neighbors in an arbitrary order. In such an approach the layout of atoms and bonds in the diagram will not result in a layout that reflects instances of chemical symmetry in the chemical structure. To sum up, "laying out symmetrically equivalent atoms and bonds in [a] chemical structure diagram in accordance with the identified symmetry," as required by claim 1, is not anticipated by the Helson thesis, because in so far as that reference discusses symmetry, it only with regard to perception, not with regard to layout.

The Examiner draws our attention to page 246, Fig. 4.5 (Chapter 4), and to Chapter 3 of the Helson thesis. But nowhere in these passages and Figure, nor anywhere else in the Helson thesis for that matter, is there any mention whatsoever of laying out symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry, as required by claim 1. Instead, the referenced passages and Figure discuss how the computer program called CAMEO (Computer Assisted Mechanistic Evaluation of Organic Reactions) described in the Helson thesis perceives symmetry in an organic molecule. But CAMEO's symmetry perception is not used to lay out a chemical structure diagram. Instead, the program uses perception of symmetry for a number of purposes that have nothing to do with laying out atoms in a diagram. First, it makes CAMEO much more efficient:

> Symmetry is common in organic chemistry and failing to detect it can mire a program in a bog of redundant processes. In Eq. 1 the failure to recognize symmetry necessitates the examination of four equivalent addition sites. Not only are three redundant reactions analyzed and a redundant intermediate created from each, but furthermore all of the intermediates themselves are carried on to further reaction, leading to a cascade of redundant structures from each cycle of processing." (page 234, lines 13-19)

Second, without symmetry perception, the number of possible structures to be examined can diverge, causing the program to fail:

> ...another problem that arises when symmetry goes unrecognized is that the number of structures in the synthesis tree can grow exponentially, a situation known as "tree explosion." Before symmetry information was available, the Radical Module would routinely "blow up" when symmetric structures of moderate complexity were submitted." (page 234, lines 20-25)

Third, symmetry perception enables CAMEO to identify identical products:

> Before we had a procedure to identify identical structures in CAMEO, our users were regularly subjected to a parade of duplicate products marching across their computer screens. With the advent of symmetry perception, most duplicate products are avoided entirely... (page 234 line 26 – page 235 line 2)

Thus, as the Helson thesis makes clear, symmetry perception addresses several important problems to do with efficiency and avoidance of redundancy, none of which have anything to do with laying out atoms in a chemical structure diagram.

The Examiner also draws our attention to Chapter 3 of the Helson thesis, entitled "Structure Diagrams from Connection Tables." To the extent Chapter 3 of the Helson thesis discusses symmetry at all, it is with regard to symmetry perception, not "laying out symmetrically equivalent atoms ... in accordance with [an] identified symmetry," as required by claim 1. Chapter 3 discusses a repositioning algorithm, which is concerned with placing molecules so that they are evenly distributed on the screen. The only inputs to the repositioning algorithm are the display screen's dimensions, referred to as the drawing window, and the dimensions of the smallest enclosing rectangle, or "box" for each molecule/ion to be placed (page 174, ¶ 3). The algorithm operates at the level of the structure diagram itself, and makes no reference whatsoever to an identified structural symmetry in a connection table for the molecule. The only reference to symmetry in Chapter 3 concerns estimating the visual appeal of an existing drawing. Quoting from Chapter 3:

> Perhaps the hardest aesthetic attribute to detect algorithmically is balance: the symmetrical distribution of like groups, and also the even distribution of white space. ...
>
> The obvious way to assess graphical symmetry would be to check if topologically equivalent atoms occupied "graphically equivalent" positions, whatever that would mean. Although this route would be preferable if it could be developed, a crude but expedient alternative has been worked out. A molecule's "graphical moment" is defined to be the vector from the midpoint of the smallest rectangle that encloses the molecule to the average atomic position. ... In effect, the moment measures how unsymmetrically the atoms are allocated within the molecular box. (page 207 line 10 – page 208 line 14)

In other words, symmetry is assessed in a pre-existing diagram in which the atoms and bonds have already been laid out. The symmetry assessment is passive, i.e., it is not used as an input to the repositioning algorithm, nor is symmetry used actively in any way as part of the process for laying out atoms and bonds. Thus nowhere does the repositioning algorithm lay out atoms and bonds in accordance with chemical structural symmetry identified in the chemical structure, such as that identified from a connection table, as required by claim 1.

In his discussion of Applicant's arguments with respect to the art, at page 13, ¶ 29 of the Office action dated August 9, 2007, the Examiner cites pages 4 and 5 of the Introduction to the Helson thesis. We assume the Examiner is drawing our attention to the following passages:

> 2) Perception of configurational symmetry of organic molecules
> ...
> 4) Structure diagram generation, i.e., the construction of conventional two-dimensional representations of organic molecules from their connection tables. (pages 4-5)

With regard to item 2), as discussed above, perception of configurational symmetry does not in any way refer to or include laying out atoms and bonds in a structure diagram based on symmetry identified in a connection table; furthermore, as previously noted, perception of symmetry serves a number of important roles that have nothing to do with structure diagram generation. With regard to item 4), the Helson thesis discusses structure diagram generation from connection tables, but it does not "identif[y], from a connection table for chemical structure, an instance of chemical structural symmetry in the chemical structure; [and] lay out... symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry..." as required by claim 1. [emphasis added]

The Examiner also cites the following passage:

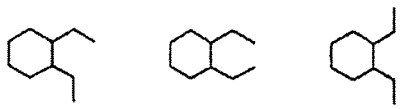
> Implementation in CAMEO
>
> In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. (last paragraph, page 145) [emphasis supplied by Examiner]

As previously discussed, repositioning does not involve "identifying, from a connection table for chemical structure, an instance of chemical structural symmetry in the chemical

structure; ... [and] laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry..." as required by claim 1. The symmetry involved here is purely to assess a diagram that is already laid out, and plays no role at all in the laying out of atoms and bonds in a chemical structure diagram.

The following examples from the Helson thesis further help to explain the distinction:

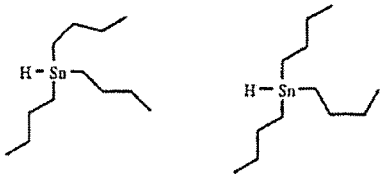
> Consider o-diethylbenzene (Fig. 3.40). In drawing A the alkyl chains are unsymmetrical ... while both drawings B and C are symmetrical, and look better for it.



	A	B	C
Moment:	105°, mag 8	—, mag 0	0°, mag 5
Magn / Alignment scores:	92 / 0	100 / 100	95 / 100
Symmetry Criterion:	69	100	96
Overall AeF score:	96	100	99

Figure 3.40. Symmetry criterion for o-diethylbenzene

> Similarly, tributyl tin hydride looks better when its chains are symmetrically directed. (Fig. 3.41, B) than otherwise (A). (Pages 207-209, emphasis added)



	A	B
Moment:	92°, mag 4	223°, mag 2
Magn / Alignment scores:	96 / 100	98 / 50
Symmetry Criterion:	96	98
Overall AeF score:	98	99

Figure 3.41. Symmetry criterion for Bu_3SnH

In other words, as these examples show, the Helson thesis assesses the impact of symmetry on the aesthetics of an existing chemical structure diagram. The discussion in the symmetry section of Chapter 3 of the Helson thesis (pages 207-209) concerns the development of a measure of graphical symmetry in a diagram that correlates to the diagram's aesthetic qualities. But it does not mention using symmetry to lay out a diagram, as required by the claim.

Next, the Examiner cites passages from Chapter 3, pages 208-209, of the Helson thesis that describe using symmetry considerations to evaluate the appearance of structure diagrams. We discussed these passages above. To summarize, the repositioning algorithm does not make any reference to, or use chemical structural symmetry inherent in the molecule, such as that identified from a connection table, as required by claim 1.

The Examiner also refers to "Algorithm 3.6 Dynamic Repositioning Engine" (page 193) from the Helson thesis. This algorithm refers to adjusting the positions of the elements of a chemical structure diagram based on the size of the drawing area, and the size of the smallest "box" that fits around each of the molecules to be drawn. Symmetry is not one of the inputs to this algorithm. Thus, the repositioning process has nothing to do with laying out symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with chemical structural symmetry identified in the chemical structure.

For the reasons discussed above, the Helson thesis does not anticipate Claim 1. Claims 5 and 9 have comparable limitations to those of claim 1, and therefore these claims, as well as the claims that depend from claims 1, 5, and 9, are also not anticipated.

Rejection of Claims under 35 U.S.C. § 103

The Examiner rejected claim 1 under 35 U.S.C. § 103(a) as being unpatentable over Hu, et al., *Chemometrics and Intelligent Laboratory Systems*, 1/18/1999 (abstract) ("Hu"), or Shelley, et al., *J. Chem. Info. Comput. Sci.*, p. 247 (1979) ("Shelley"), or Fan et al., *J. Chem. Info. Comput. Sci.*, pp. 654-59 (1996) ("Fan") in view of the Helson thesis.

The Examiner admits that Hu or Shelley or Fan do not disclose positioning atoms and bonds in a chemical structure diagram. To supply that which is missing, the Examiner turns to Helson, and repeats his belief that the Helson thesis discloses "positioning in chapter 3 (CAMEO) of symmetrical structures (Chapter 4)." But that is not correct, as we show in the discussion above in response to the rejections under § 102. Nowhere in Chapter 3, nor anywhere else in the Helson thesis for that matter, does Helson even hint at using his system to position symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with a chemical structural symmetry identified in the connection table of the chemical structure.

Hu *et al.*, Shelley *et al.* or Fan does not cure this deficiency because the role of symmetry in these references is a passive one, rather like that disclosed in the Helson thesis, in contrast to the claimed active role played by symmetry in laying out a chemical structure diagram. As previously explained in the Response to Office Action dated May 24, 2006, Hu is concerned with the detection of topological symmetry, in a chemical structure, not the expression of such symmetry in a chemical structural diagram. Shelley, like Hu, teaches an algorithm for detecting topological symmetry. Similarly, Fan, like Hu and Shelley, is concerned with the detection of equivalent atoms: "A simple and efficient algorithm for the perception of constitutionally equivalent atoms in a target molecule is reported." (page 654, abstract, emphasis added) None of these references teaches or suggests laying out symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with a symmetry identified in a connection table for the chemical structure. Thus, the cited references, either separately, or taken in combination, fail to teach or even suggest all the elements of the claim.

The Examiner asserts that in Applicant's Response dated May 21, 2007, Applicant made a piecemeal argument, and that one cannot show non-obviousness by attacking references individually where the rejections are based on combinations of references. However, in the present case, the cited references taken in combination fail to teach or suggest an element of the claim. The Examiner argues that the missing element is disclosed in the Helson thesis, but as we explain above, that is not the case. The Examiner has provided no reason or pointed to any teaching or suggestion as to why the missing element is supplied by any of the other cited references, or that the missing element should be known to a person of ordinary skill in the art. Furthermore, as we discuss above, the symmetry perception step does not itself in any way involve, teach, or suggest "identifying, from a connection table for chemical structure, an instance of chemical structural symmetry in the chemical structure; ... [and] laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry..." as required by claim 1.

Accordingly, Applicant submits that claim 1 is not obvious in view of Hu or Shelley, or Fan, further in view of the Helson thesis. Claims 5 and 9, which have analogous limitations to those of claim 1, as well as the claims that depend from claims 1, 5, and 9, are also not obvious over the cited references. Likewise, new claims 28-35 include identifying an instance of

chemical structural symmetry in a chemical structure and laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry.

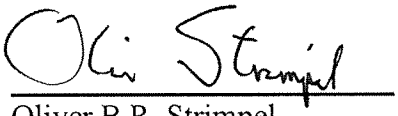
CONCLUSION

In view of the above, Applicant believes the pending application is in condition for allowance.

Please charge any other fees that may be due, or credit any overpayments to our Deposit Account No. 08-0219, under Order No. 0103544.00131US2 from which the undersigned is authorized to draw.

Respectfully submitted,

Dated: October 29, 2007



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